Development of High-Fidelity and Efficient Modeling Capabilities for Enabling Co-Optimization of Fuels and Multi-Mode Engines

Project ID: ace152

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2020 Annual Merit Review

U.S. Department of Energy's (DOE) Vehicle Technologies Office

Stanford University | UCONN | University of Connecticut | Argonne National Laboratory

Overview

Timeline

- Project start: 10/01/2019
- Project end: 9/30/2022
- Percent complete: <15%

Project Partners:

- University of Connecticut: Prof. T. Lu
- Argonne National Lab: Drs. P. Pal, M. Ameen

Budget:

- Year 1: $424,172 DOE/$99,845 Cost-share
- Stanford: $224,172 DOE/$66,845 Cost-share
- University of Connecticut : $100,000 DOE/ $33,000 Cost-share
- ANL: $100,000

Barriers

- Co-optimization of fuel and engine
- Extend lean-combustion to intermediate and high-load conditions
- Investigation of new ignition systems
- Improve understanding and modeling of multimode combustion and emissions formation, as well as their interaction with chamber/piston geometry

Relevance

Impact

- Co-optimization of fuels and engines has potential for significant gains in engine performance and efficiency
- Extension of operating condition to high-load range through multi-mode combustion regimes and spark-assisted compression ignition
- Need for accurate and reliable high-fidelity modeling tools to enable successful implementation, control, and optimization of multi-mode combustion regimes, high-energy ignition processes, and wall-heat transfer

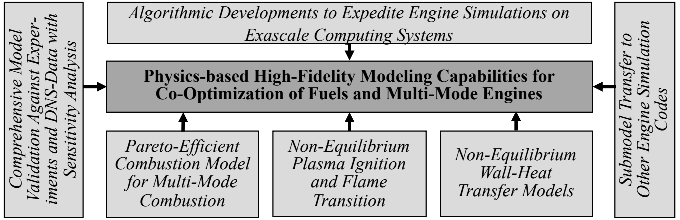
Objectives: Develop improved physical models and numerical algorithms to enable reliable predictions of multi-mode combustion to support EERE's Co-Optima program

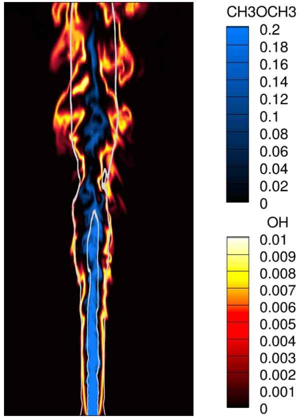
- Develop accurate submodels for predicting multi-mode combustion regimes, wall-heat transfer, ignition, and combustion-mode transition
- Develop numerical algorithms and efficient time-integration schemes for exascale computing
- Validate computational submodels against experiments and DNS data

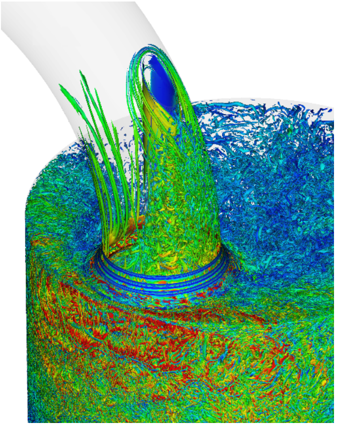
Approach

Develop improved physical models and numerical algorithms for predicting multi-mode combustion

- **Task 1 – Pareto-efficient combustion model for multi-mode combustion:** fidelity-adaptive combustion-modeling framework that utilizes dynamic submodel assignment for prediction of complex multimode combustion regimes under consideration of requirements on quantities of interest, accuracy, and computational cost
- **Task 2 – High-energy ignition modeling**
  - Chemical Explosive Mode Analysis to identify local combustion modes and flame structures
  - Develop skeletal & reduced models using DRG; DRG-aided SA to obtain minimal skeletal models for given accuracy requirements
- **Task 3 – Non-equilibrium wall-heat transfer model** for prediction heat-transfer in ICEs
- **Task 4 – Multi-mode engine simulations on exascale platform with Nek5000**
  - High-order leads to exponential convergence
  - Proven high scalability on up to 10^6 processors



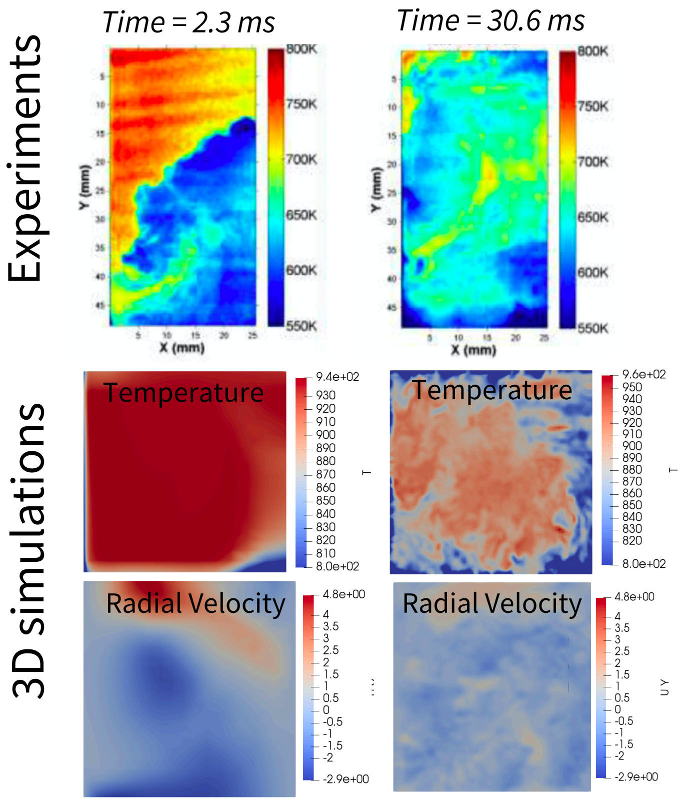




Technical Accomplishments and Progress (Stanford)

Task 1: Multimode combustion modeling

- Simulation of multimode RCM (Strozzi 2008/2019)
- Challenges: flow heterogeneity by piston impacts ignition characteristics, moving geometry
  - Generate time-dependent boundary conditions from pre-calculated Fluent simulation
  - Dynamic grid capability in CharLESX
    - LES-solver with multi-species capability
    - PEC-implementation, load-balancing
- Simulation results
  - HCCI: CH_4/Air at T = 930K, P = 44bar (TDC)
    - Ignition at 58ms, experiment: 35ms → inert compression stroke
  - SICI: CH_4/Air at T = 930K, P = 44bar (TDC)
    - Spark model: energy deposition at TDC
    - Ignition at 3.4ms

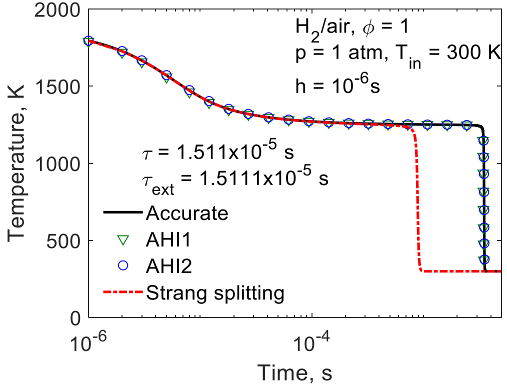


Technical Accomplishments and Progress (UConn)

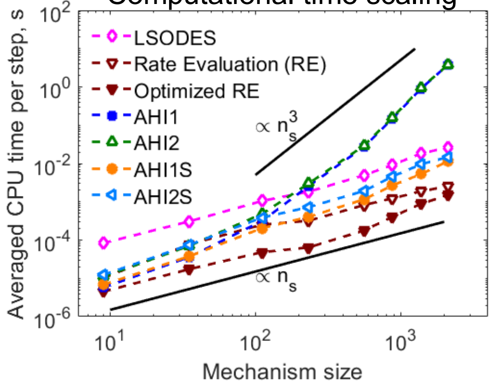
Task 2: High-energy ignition modeling

- Non-equilibrium plasma ignition involves severe stiffness - must be modeled in engine CFD
- Model to be created based on CFD of kernel growth, involves
  - Large number of species and reactions
  - Extremely short timescales for energy relaxation
  - Lack of flow/transport models
  - Previous chemistry solvers face challenges in accuracy and/or efficiency
- A novel second order dynamic adaptive hybrid integration (AHI2) scheme solver is developed to address these challenges and provide significantly improved accuracy and efficiency
- AHI2 eliminates O(1) splitting error
- Linear complexity achieved with AHIS schemes

Extinction of stirred reactor



Computational time scaling



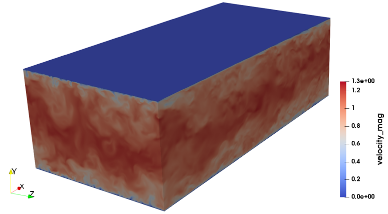
Technical Accomplishments and Progress (ANL)

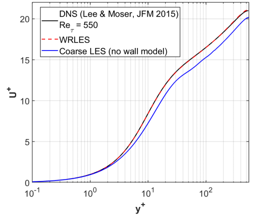
Task 3: Wall Modeling in Nek5000

- Baseline configuration of turbulent channel flow for model verification
  - Performed wall-resolved LES (WRLES) with literature DNS data to validate baseline setup
  - Implemented algebraic wall-stress model
- Next Steps: Implement non-equilibrium wall model, and validate for canonical non-equilibrium as well as IC engine flows

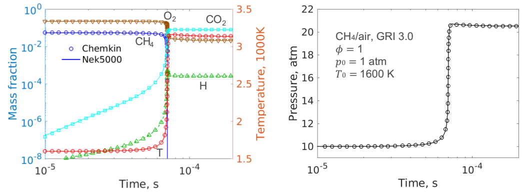
Task 4: Multi-mode engine simulations on Nek5000

- Implemented detailed chemical kinetic and molecular transport into Nek5000
- Validation of thermochemistry extension using a series of canonical reactor/flame configurations → excellent agreement with reference solutions
- New capabilities assure high-fidelity engine combustion simulations in Nek5000

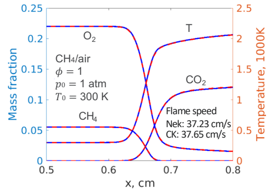




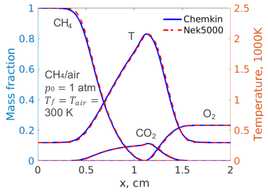
Constant pressure auto-ignition



1D premixed flame



2D counterflow non-premixed flame



Collaboration and Coordination with Other Institutions

- Ignition modeling
  - Sandia National Labs (Drs. Jackie Chen and Isaac Ekoto)
    - High-energy ignition and DNS analysis
- Nek5000 model development
  - Drs. Saumil Patel, Juan Colmenares (ANL)
  - Prof. Paul Fischer (UIUC)
- Combustion modeling
  - Sandia National Labs: DISI engine experimental data
  - Dr. Camille Strozzi (CNRS): Experimental data for multimode RCM
- Wall modeling
  - Volker Sick (U-M Ann Abror): Experimental data for TCC-III engine

Proposed Future Research

Task 1: Pareto-efficient combustion model for multi-mode combustion

- PEC-drift term formulation for multimode combustion
- Validation of PEC against multi-mode RCM

Task 2: High-energy ignition model

- High-energy discharge model; Implement plasma equations; Extend model reduction methods to plasma kinetics
- Analyze ignition model against DNS, and validate against Sandia spark calorimeter

Task 3: Non-equilibrium wall-heat transfer model

- Validation of equilibrium wall model in Nek5000
- Formulation of non-equilibrium wall model for variational spectral element method

Task 4: Multi-mode engine simulations on exascale platform

- Algorithmic developments in Nek5000
- Benchmark simulation of TCC-III engine with Nek5000

Summary

Develop improved physical submodels and numerical algorithms to enable accurate and efficient predictions of multi-mode combustion to support EERE's Co-Optima program

- Adaptive LES-combustion model utilizing Pareto-efficient combustion framework for multimode combustion and ignition transition
- Chemical reduction strategies for plasma-ignition
- Non-equilibrium wall model for prediction wall-heat transfer
- Model transition into open-source exascale Nek5000 computing platform

Technical Back-Up

Project Overview

Develop improved physical submodels and innovative numerical algorithms to enable accurate and efficient predictions of multi-mode combustion to support EERE's Co-Optima program

Task 1: Pareto-efficient combustion (PEC) model for multi-mode combustion

- Develop fidelity-adaptive combustion model for reliably predicting multi-mode combustion under consideration of user-specific requirements about quantities of interest, solution accuracy and computational cost
- Validate resulting PEC-formulation in multi-mode engine simulations and implemented into Nek5000 for integrated exascale engine simulations
- PEC is a trust-region formulation that utilizes a drift term to assess the local combustion-model compliance

Task 2: High-energy ignition model for predicting non-equilibrium plasma ignition and flame-mode transition

- Develop high-energy plasma ignition model that combines local combustion-mode identification with adaptive chemistry
- Integrate ignition model into PEC-framework
- Develop reduced plasma-kinetic models by extending existing chemical reduction techniques and utilize mode-adaptive reduced kinetics to capture transient ignition processes
- Validated against measurements and a priori DNS-analysis

Project Overview

Develop improved physical submodels and innovative numerical algorithms to enable accurate and efficient predictions of multi-mode combustion to support EERE's Co-Optima program

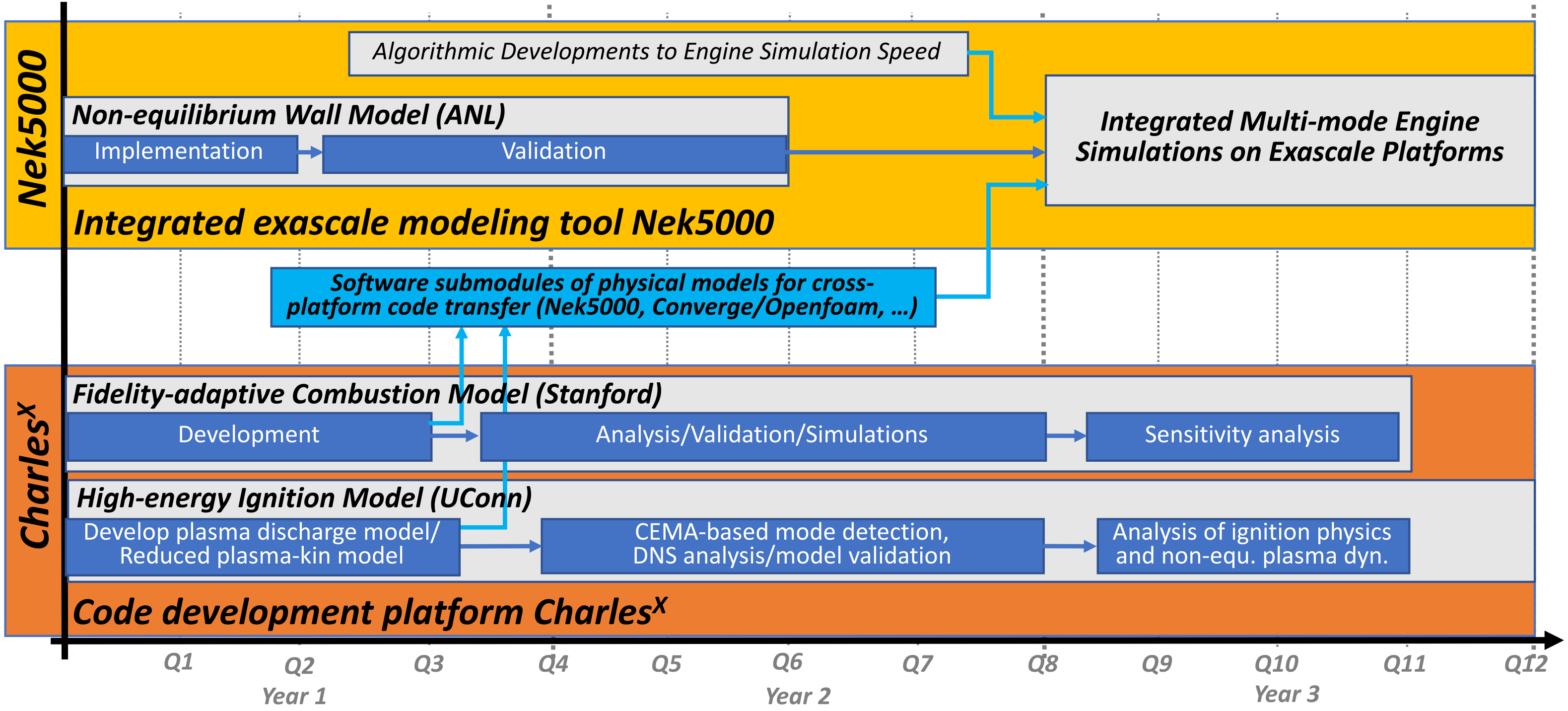
Task 3: Non-equilibrium wall-heat transfer model:

- Integrate non-equilibrium wall model (Ma et al. 2017) into Nek5000 to describe the near-wall thermo-viscous boundary layer
- Through validation against measurements and benchmark calculations, demonstrate quantitative improvements in the heat-transfer predictions at comparable cost and robustness

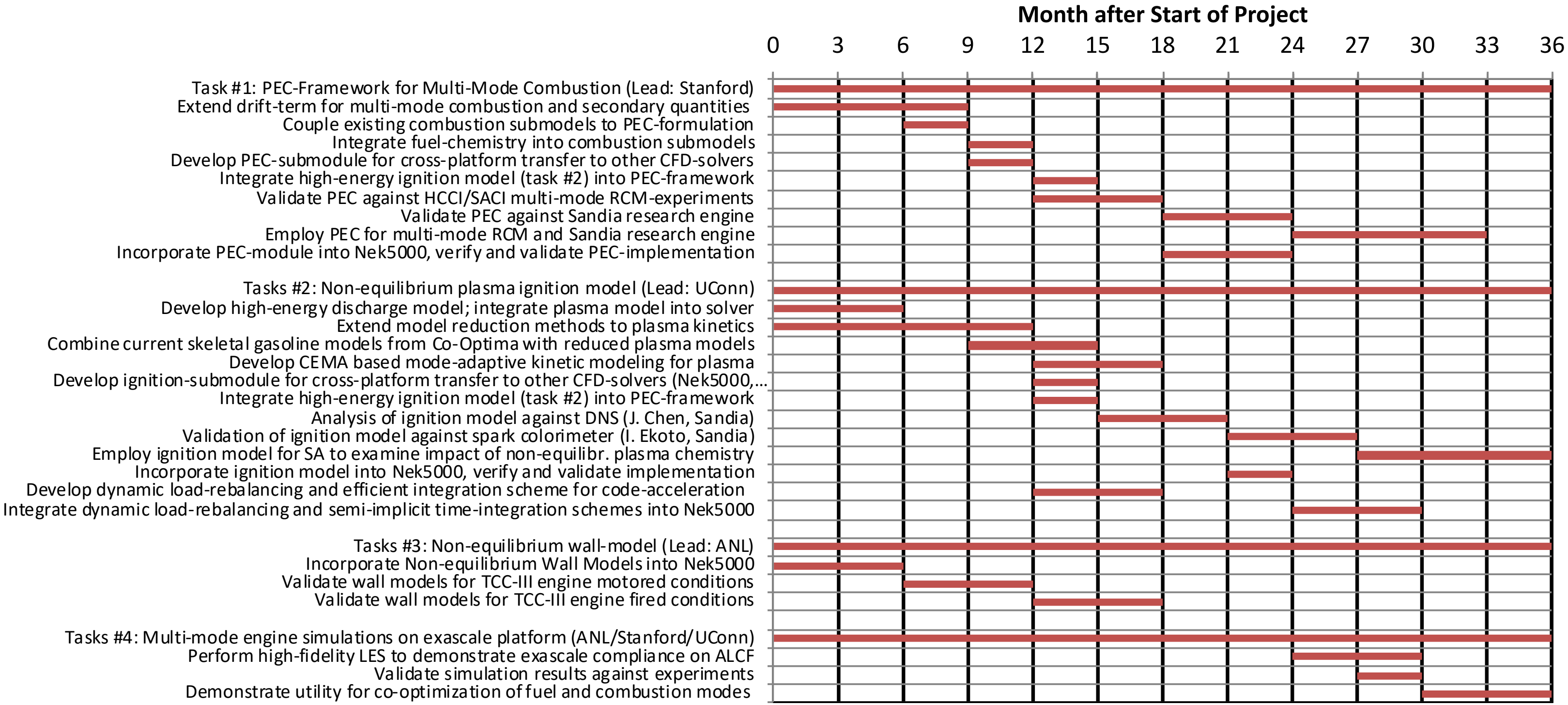
Task 4: Multi-mode engine simulations on exascale platform

- Perform comprehensive validation to examine the accuracy and address deficiencies of individual submodels
- Consider experiments for (i) multi-mode rapid compression engine, (ii) Sandia spark calorimeter, (iii) U. of Michigan transparent combustion chamber (TCC)-III engine, (iv) Sandia research engine
- Model transition into Nek5000 to perform integrated exascale simulations of engine experiments established under Co-Optima program

Project Plan and Software Platform



Project Schedule

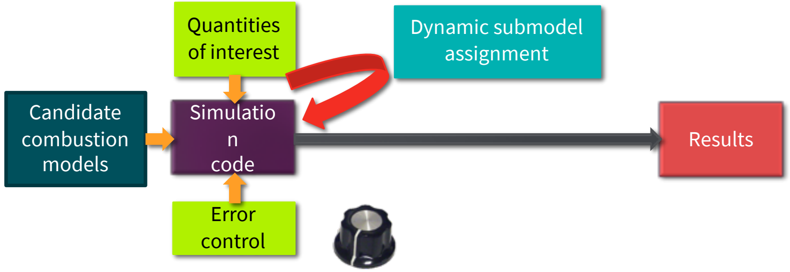


Background and Related Research

Pareto-Efficient Combustion (PEC) Model

Pareto-efficient combustion framework to enable optimal submodel assignment, under consideration of user-specific input about

- Quantities of interest
- Set of combustion submodels
- Desired accuracy and cost



PEC input parameter

- Set of quantities of interest: $Q = \{Y_{CO2}, Y_{CO}, Y_{H2O}, Y_{NO}, \ldots\}$
- Set of candidate combustion models: M
- Penalty term λ for cost/accuracy trade-off

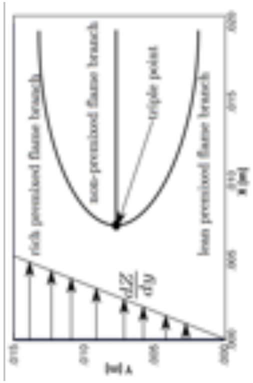
Model Problem: Tribrachial Flame

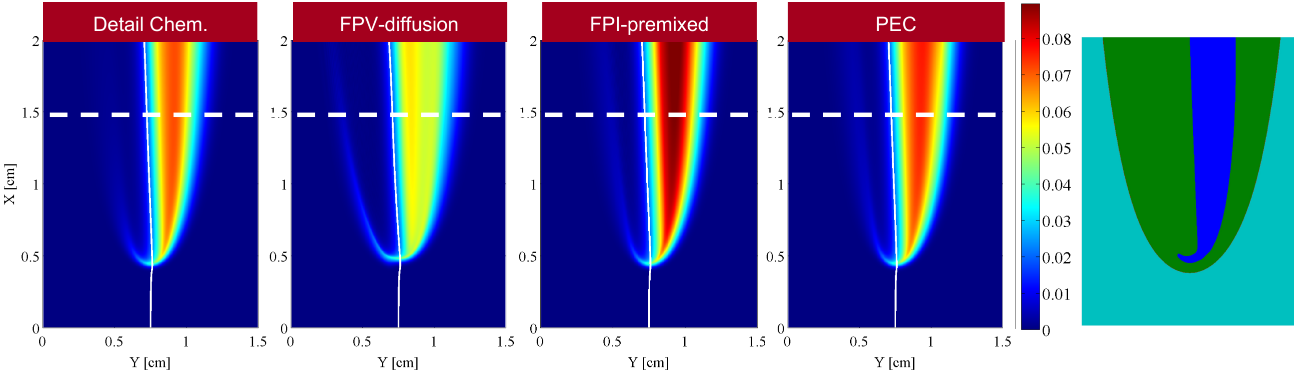
Configuration

- CH4-Air laminar flame
- Stratification of reactants

PEC-model setup

- *M = {DC, FPV, FPV, IM},*
- *Q={CO2, CO, H2O, H2, NO}, λ = 0.2*





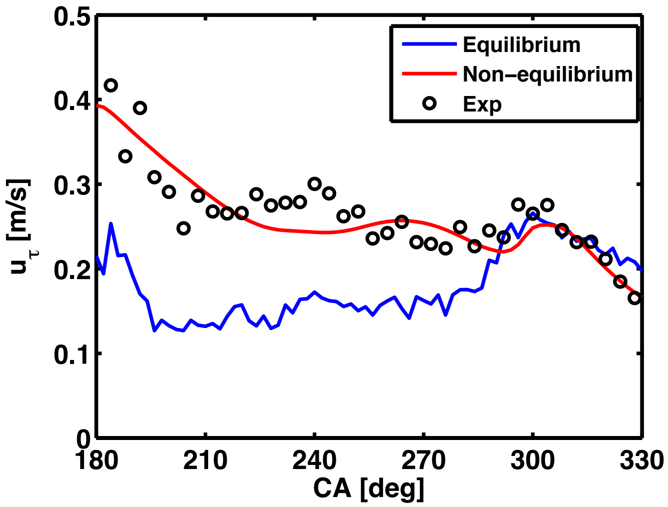
Non-equilibrium Wall Heat Transfer Model

- Equilibrium wall model – Algebraic wall-function model

$$u^+ = \begin{cases} y^+ & \text{if } y^+ < 11 \\ \frac{1}{\kappa}\ln y^+ + B & \text{if } y^+ \geq 11 \end{cases}$$

- Non-equilibrium wall model (with pressure gradient)

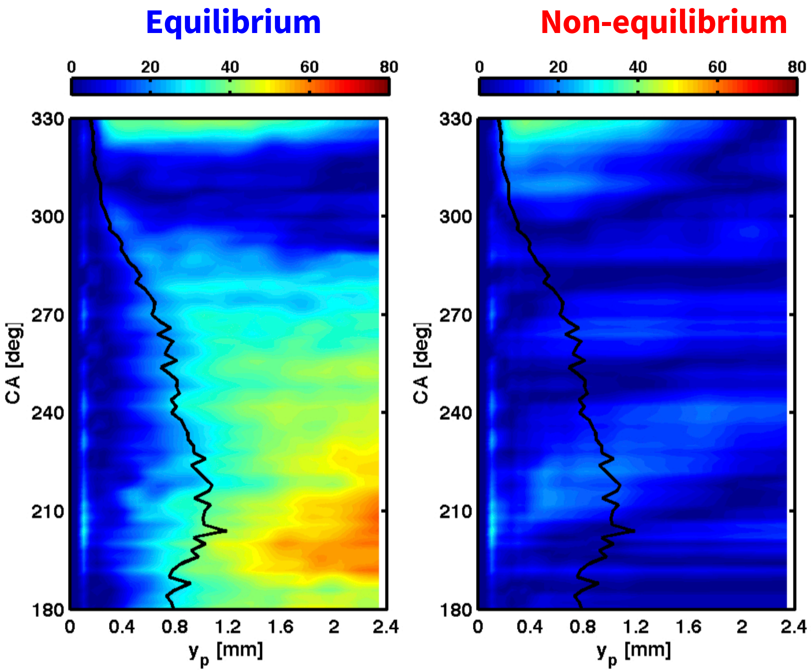
$$\frac{\partial \bar\rho}{\partial t} + \frac{\partial}{\partial y}(\bar\rho \bar v) = 0\,,$$
$$\bar\rho \frac{\partial \bar u}{\partial t} + \bar\rho \bar v \frac{\partial \bar u}{\partial y} = \boxed{-\frac{\partial \bar p}{\partial x}} + \frac{\partial}{\partial y}\left((\bar\mu + \mu_t)\frac{\partial \bar u}{\partial y}\right)\,,$$
$$\bar\rho c_p \frac{\partial \overline{T}}{\partial t} + \bar\rho c_p \bar v \frac{\partial \overline{T}}{\partial y} = \frac{\partial \bar p_0}{\partial t} + \frac{\partial}{\partial y}\left((\overline{\lambda} + \lambda_t)\frac{\partial \overline{T}}{\partial y}\right)\,,$$
$$\bar p_0 = \bar\rho R \overline{T}\,,$$



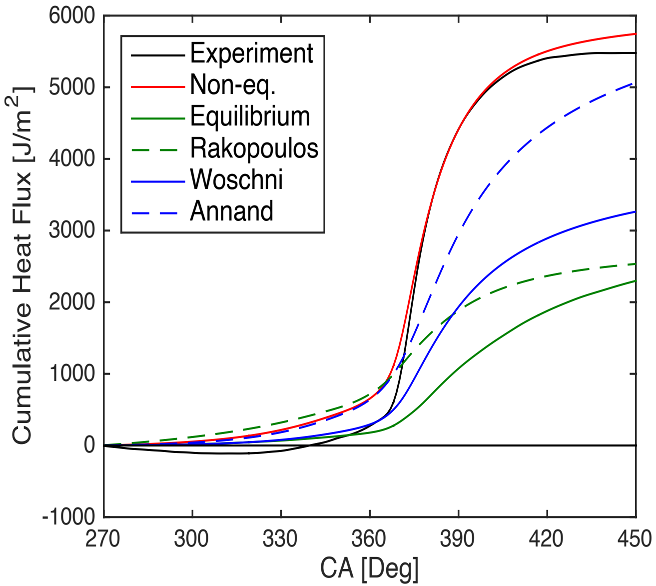
Non-equilibrium Wall Heat Transfer Model

Prediction of shear velocity

$$(u_\tau - u_\tau^{exp})/u_\tau^{exp}$$



Prediction of wall heat flux



Chemical Explosive Mode Analysis (CEMA)

Transport equations for a general reacting flow

$$\frac{D\mathbf{y}}{Dt} = \mathbf{g}(\mathbf{y}) = \boldsymbol{\omega}(\mathbf{y}) + \mathbf{s}(\mathbf{y})$$

y: the vector of variables (e.g. species concentrations and temperature)
ω: chemical source term
s: other source terms (e.g. diffusion)

Zero-crossing of λ_e (1st eigenvalue of the chemical Jacobian):

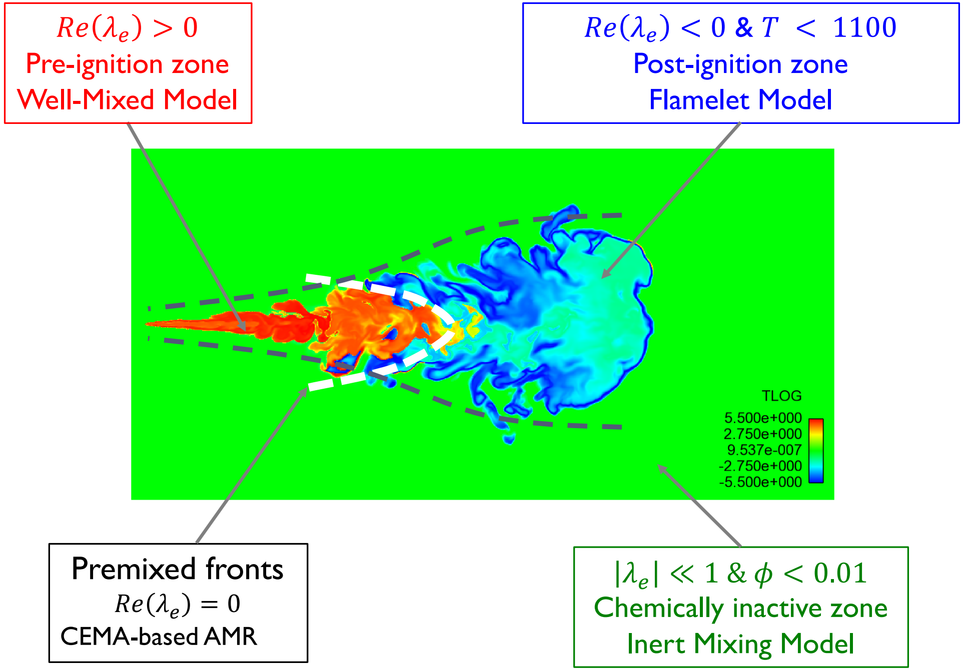
- Transition between reactants ($\lambda_e > 0$) and products ($\lambda_e < 0$)
- Ignition state in auto-ignition
- Extinction state in continuous flow reactors
- Reaction zone locations in premixed flames

CEMA is a robust diagnostic for local combustion modes and global flame structures (both premixed and non-premixed)

CEMA-based Flame Segmentation and Dynamic Modeling

A lifted Spray-A flame (diesel condition)

- LES with CONVERGE v2.3
- CEMA-based flame zone segmentation
- Dynamic adaptive modeling for different zones
- Implemented as a CONVERGE UDF

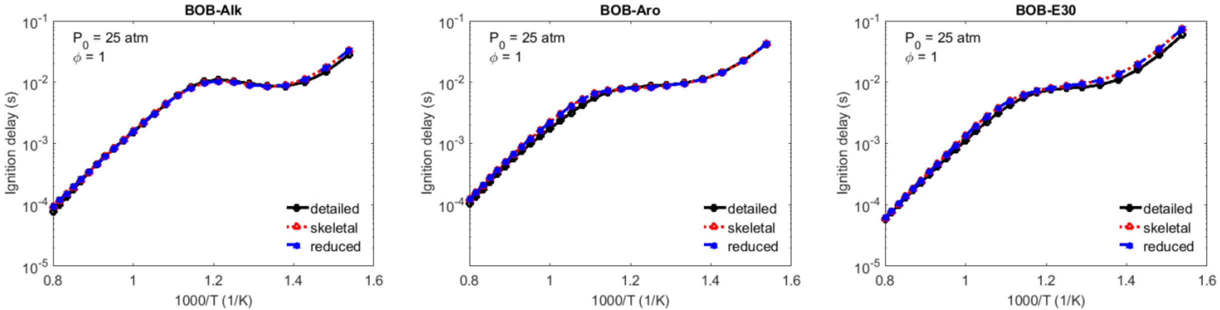


(Xu et al, CNF 2018)

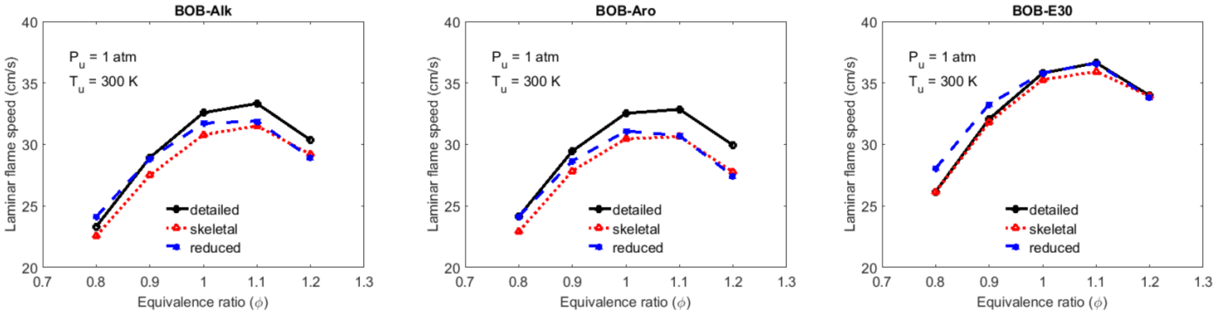
Sample Validation of the Reduced Kinetic Models

Fuel surrogate	i-C8H18 (vol%)	n-C7H16 (vol%)	C6H5CH3 (vol%)	C6H12-1 (vol%)	C2H5OH (vol%)	n-C5H12 (vol%)	i-C5H12 (vol%)	C4H10 (vol%)	1,2,4-TMB (vol%)
BOB-Alk	93	-	-	-	-	4	-	1	2
BOB-Aro	42	-	11	5	-	9	6	5	22
BOB-E30	26.6	11.9	-	4.9	30	8.4	7.7	2.8	7.7

Ignition delay



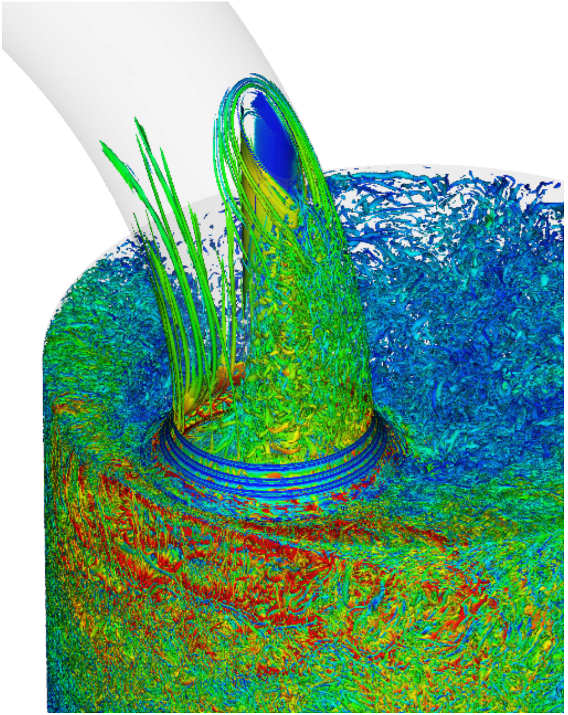
Flame speed



Nek5000 for High-Fidelity Engine Simulations

Nek5000 is a spectral element code that has been under active development for 30+ years

- High-order leads to exponential convergence
- Proven high scalability on up to 106 processors
- Written in Fortran and C
- Pure MPI for parallelization



Applications span a wide range of fields, including fluid flow, thermal convection, combustion and magnetohydrodynamics

Current version can handle low-Mach and incompressible flows; compressible version under validation

Currently funded by DOE VTO at ANL to enable high-fidelity IC engine simulations on upcoming exascale platforms

Spray and combustion models are being implemented into Nek5000 as part of the DOE VTO project